SECOND LAW, DETAILED BALANCE AND LINEAR MARKOVIAN DYNAMICS DETERMINE SHANNON ENTROPY

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"STOCHASTIC THERMODYNAMICS IN COMPLEX SYSTEMS"

CSH ONLINE WORKSHOP

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IN THIS TALK, WE WILL EXPLORE THE RELATIONSHIP BETWEEN TWO ASPECTS OF THERMODYNAMICS:

A) STOCHASTIC THERMODYNAMICS

B) GENERALIZED ENTROPIES

A) STOCHASTIC THERMODYNAMICS

- EMERGENT FIELD OF THERMODYNAMICS (SINCE 90'S)
- DESCRIBES NON-EQULIBRIUM THERMODYNAMICS BY STOCHASTIC VARIABLES, ESPECIALLY IN MICROSCOPIC SYSTEMS
- MAIN RESULTS (OTHER TALKS): FLUCTUATION THEOREMS, THERMODYNAMIC UNCERTAINTY RELATIONS, NANOMOTORS…

A) STOCHASTIC THERMODYNAMICS

KEY ASPECTS

1) MASTER EQUATION: *LINEAR MARKOVIAN DYNAMICS*

$$\dot{p}_m = \sum_n (w_{mn} p_n - w_{nm} p_m)$$

2) (LOCAL) DETAILED BALANCE: *PROBABILITY CURRENTS VANISH FOR (LOCAL) EQUILIBRIUM DISTRIBUTIONS*

$$\frac{w_{mn}}{w_{nm}} = \frac{p_m^\star}{p_n^\star} = \exp\left(-\frac{\epsilon_m - \epsilon_n}{T}\right)$$

3) SECOND LAW OF THERMODYNAMICS:

$$\dot{S} \geq \frac{\dot{Q}}{T}$$

B) GENERALIZED ENTROPIES

- STUDIED IN INFORMATION THEORY SINCE 60'S
- USED IN PHYSICS SINCE 90'S
- MAIN AIM: STUDY THERMODYNAMICS OF SYSTEMS WITH NON-BOTLZMANNIAN EQUILIBRIUM DISTRIBUTIONS (DUE TO CORRELATIONS, LONG-RANGE INTERACTIONS…)

B) GENERALIZED ENTROPIES

KEY ASPECTS

I.) GENERAL FORM OF ENTROPY:

$$S(P) = f\left(\sum_m g(p_m)\right)$$

II.) MAXIMUM ENTROPY PRINCIPLE:

Maximize S(p) subject to constraint that p is normalized and expected energy has a given value

Solution: MaxEnt distribution: $p_m^\star = (g')^{-1}\left(\frac{\alpha+\beta\epsilon_m}{C_f}\right), \quad C_f = f'(\sum_m g(p_m))$

QUESTION: FOR WHAT GENERAL FORM OF ENTROPIES DO THE KEY ASPECTS OF STOCHASTIC THERMODYNAMICS HOLD IF THE SYSTEM IS OFF EQUILIBRIUM?

REQUIREMENTS

BLUE - STANDARD STOCHASTIC THERMODYNAMICS

0) DEFINITIONS

INTERNAL ENERGY

$$U = \sum_m p_m \epsilon_m$$

ENTROPY

$$S = f\left(\sum_m g(p_m)\right)$$

$$S = -\sum_m p_m \log p_m$$

1) MARKOVIAN DYNAMICS

$$\dot{p}_m = \sum_n \left[J(w_{mn}, p_n) - J(w_{nm}, p_m)\right]$$

$$\dot{p}_m = \sum_n (w_{mn}p_n - w_{nm}p_m)$$

NORMALIZATION

$$\sum_m \dot{p}_m = 0$$

TRANSITION RATES

$$w_{mn}$$

PROBABILITY CURRENTS

$$\left[J(w_{mn}, p_n) - J(w_{nm}, p_m)\right]$$

2) DETAILED BALANCE

TWO WAYS HOW TO CHARACTERIZE EQUILIBRIUM:

A) MAXIMUM ENTROPY PRINCIPLE

$$p_m^\star = (g')^{-1}\left(\frac{\alpha+\beta\epsilon_m}{C_f}\right)$$

$$p_m^\star = \exp(-\alpha - \beta\epsilon_m)$$

B) PROBABILITY CURRENTS VANISH

$$J(w_{mn}, p_n^\star) = J(w_{nm}, p_m^\star)$$

$$w_{mn}p_n^\star = w_{nm}p_m^\star$$

3) SECOND LAW OF THERMODYNAMICS

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \dot{S}_i + \dot{S}_e$$

ENTROPY PRODUCTION RATE

$\dot{S}_i \geq 0$ and $\dot{S}_i = 0 \Leftrightarrow J(w_{mn}, p_n) = J(w_{nm}, p_m) \; \forall \; m, n$

ENTROPY FLOW RATE

$\dot{S}_e = \frac{1}{T} \sum_m \dot{p}_m \epsilon_m = \frac{\dot{Q}}{T}$

MAIN RESULT

THEOREM:

REQUIREMENTS 1-3) IMPLY THAT

$$J(w_{mn}, p_n) = \psi(j(w_{mn}) - g'(p_n))$$

WHERE

j - arbitrary function

ψ - increasing function

IDEA OF THE PROOF

1. CALCULATE TIME DERIVATIVE OF ENTROPY
2. DIVIDE IT INTO
   - NON-NEGATIVE ENTROPY PRODUCTION RATE
   - ENTROPY FLOW RATE
3. USE DETAILED BALANCE
4. FROM ENTROPY FLOW RATE WE GET CONSTRAINTS ON THE FORM OF THE CURRENT
5. PROOF IN THE APPENDIX (AVAILABLE ON WEB)

EXAMPLES

LINEAR MARKOVIAN DYNAMICS

$$\dot{p}_m = \sum_n (w_{mn} p_n - w_{nm} p_m)$$

$$J_{mn} = w_{mn} p_n = \exp(\log w_{mn} + \log p_n)$$

$$\Rightarrow g'(p_n) = -\log(p_n)$$

$$\Rightarrow S = -\sum_n p_n \log p_n$$

REQUIRING SECOND LAW, DETAILED BALANCE, AND LINEAR MARKOVIAN DYNAMICS FORCES ENTROPY TO BE SHANNON ENTROPY

FINITE HEAT BATH

HAMILTONIAN: $H = H_{system} + H_{bath}$

SCALING: $\lambda H_{bath}(x_1, \ldots, x_n) = H_{bath}(\lambda^{1/a_1} x_1, \ldots, \lambda^{1/a_n} x_n)$

EQUILIBRIUM: $p(E) \propto \int \delta(E - H_{bath})\, \mathrm{d}x_1 \ldots \mathrm{d}x_n$

Q-EXP: $p(E) \propto (1 - (q-1)\beta E)^{1/(q-1)}$

TSALLIS ENTROPY: $S = \frac{1}{1-q}(\sum_m p_m^q - p_m)$

$$\Rightarrow g'(p_m) = \frac{q p_m^{q-1} - 1}{1-q}$$

MASTER EQUATION: $J_{mn} = \psi(j(w_{mn}) + \frac{q p_m^{q-1} - 1}{q-1})$

FINITE HEAT BATH CONSEQUENCES

REASONABLE SCENARIOS

IF ALL REQUIREMENTS ARE OBEYED

SYSTEM'S DYNAMICS IS NON-LINEAR

IF ALL REQUIREMENTS EXCEPT 1) ARE OBEYED

SYSTEM'S DYNAMICS IS NON-MARKOVIAN

FINITE HEAT BATH CONSEQUENCES

UNREASONABLE SCENARIOS

IF ALL REQUIREMENTS EXCEPT 2) ARE OBEYED

THEN THE DISTRIBUTION OBTAINED FROM ENTROPY MAXIMIZATION WOULD BE A NON-EQUILIBRIUM STEADY STATE

IF ALL REQUIREMENTS EXCEPT 3) ARE OBEYED

THEN SECOND LAW OF THERMODYNAMICS WOULD BE VIOLATED

MAIN IDEA

NON-BOLTZMANNIAN EQUILIBRIUM DISTRIBUTION

IN A SYSTEM SATISFYING

DETAILED BALANCE AND 2ND LAW

FORCES THE SYSTEM TO OBEY EITHER

NON-LINEAR OR NON-MARKOVIAN DYNAMICS

APPENDIX
SKETCH OF PROOF

STANDARD STOCHASTIC THERMODYNAMICS

$$\dot{S} = -\sum_m \dot{p}_m \log p_m$$

$$= -\tfrac{1}{2} \sum_{mn} (w_{mn} p_n - w_{nm} p_m) \log \tfrac{p_m}{p_n}$$

$$= \underbrace{\frac{1}{2} \sum_{mn} (w_{mn} p_n - w_{nm} p_m) \log \frac{w_{mn} p_n}{w_{nm} p_m}}_{\dot{S}_i}$$

$$+ \underbrace{\frac{1}{2} \sum_{mn} (w_{mn} p_n - w_{nm} p_m) \log \frac{w_{mn}}{w_{nm}}}_{\dot{S}_e}$$

$$= \dot{S}_i + \dot{S}_e \geq \frac{\dot{Q}}{T}$$

SKETCH OF PROOF

$$\dot{S} = C_f \sum_m \dot{p}_m g'(p_m)$$
$$= \frac{C_f}{2} \sum_{mn} (J_{mn} - J_{nm})(g'(p_m) - g'(p_n))$$

$$= \frac{C_f}{2} \sum_{mn} (J_{mn} - J_{nm})(\Phi_{mn} - \Phi_{nm})$$
$$+ \frac{C_f}{2} \sum_{mn} (J_{mn} - J_{nm})(g'(p_m) + \Phi_{nm} - g'(p_n) - \Phi_{mn})$$

$$= \underbrace{\frac{C_f}{2} \sum_{mn} (J_{mn} - J_{nm})(\phi(J_{mn}) - \phi(J_{nm}))}_{\dot{S}_i}$$
$$+ \underbrace{\frac{C_f}{2} \sum_{mn} (J_{mn} - J_{nm})(g'(p_m) + \phi(J_{nm}) - g'(p_n) - \phi(J_{mn}))}_{\dot{S}_e}$$

SKETCH OF PROOF

$\dot{S}_i \Rightarrow \phi -\ \ increasing$

$\dot{S}_e \Rightarrow C_f[g'(p_m) + \phi(J_{nm}) - g'(p_n) - \phi(J_{mn})] = \frac{\epsilon_n - \epsilon_m}{T}$

$\Rightarrow \phi(J_{mn}) = j(w_{mn}) - g'(p_n)$

$\Rightarrow J_{mn} = \psi(j(w_{mn}) - g'(p_n))$, $\psi = \phi^{-1}$ - increasing

$\square$.

NOTES:

$j(w_{mn}) - j(w_{nm}) = \frac{\epsilon_n - \epsilon_m}{C_f T}$

$\beta = \frac{1}{T}$

ANALOGOUS FOR MULTIPLE HEAT BATHS